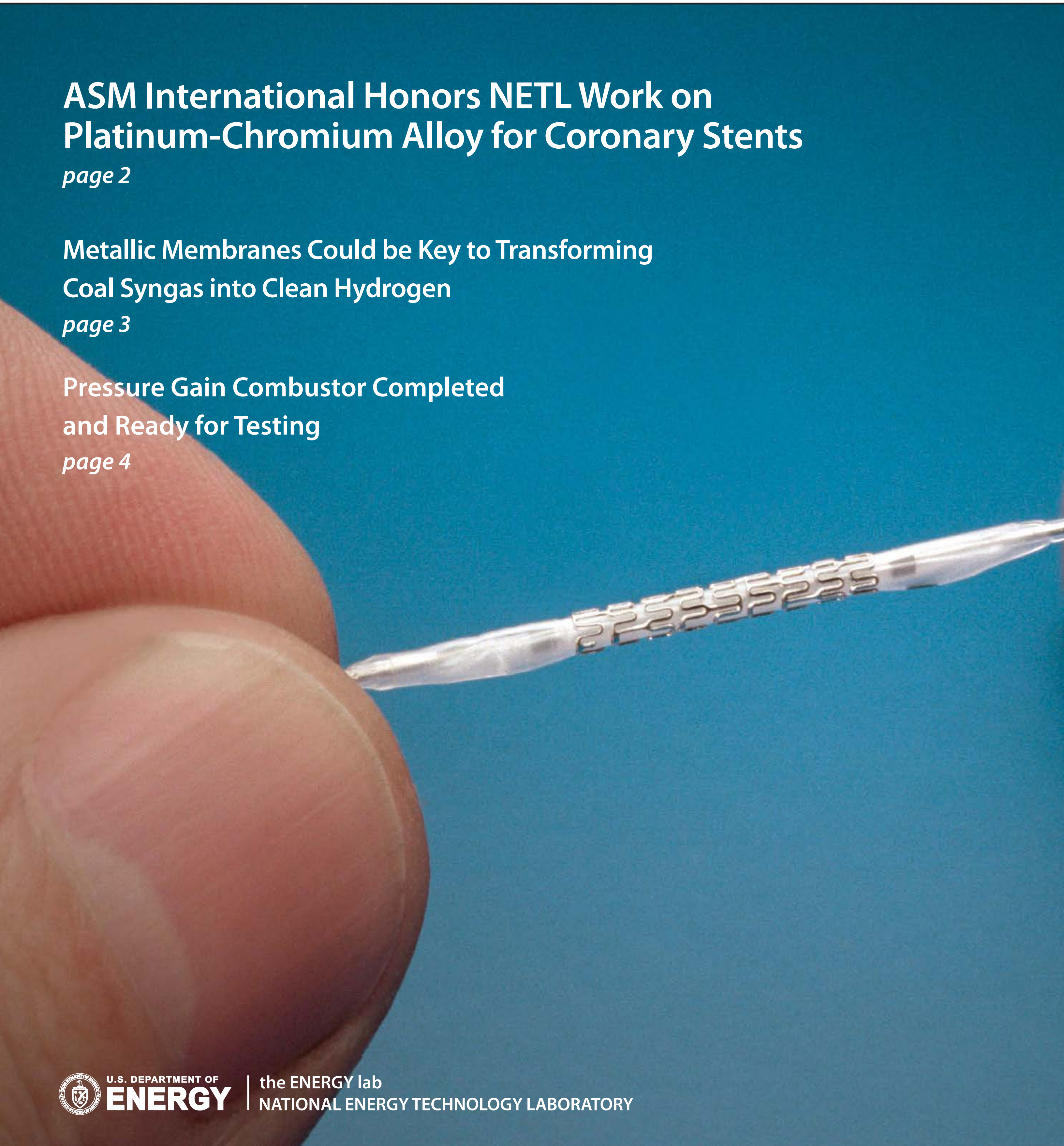
netlognews

NETL's Quarterly R&D newsletter — July 2014, Issue 34



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Cover image: *photo of a prototype coronary stent*

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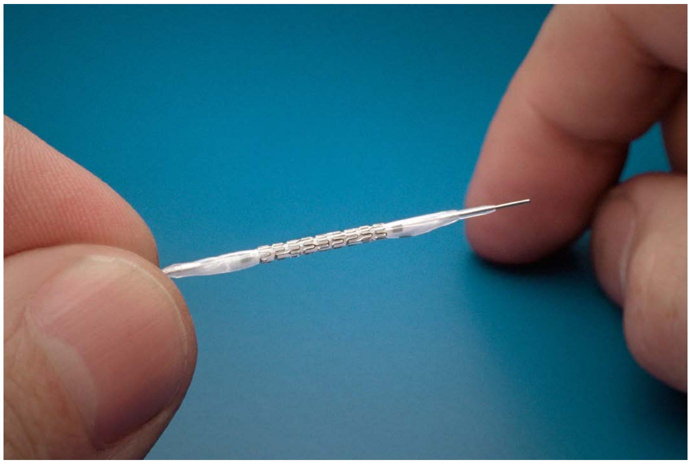
This is the final edition of Netlognews. We will be transitioning into a new, monthly NETL Research & Development newsletter beginning in October 2014. I hope you have enjoyed this newsletter about the Lab's research, and look forward to providing our new publication to you.

If you would like to be on the mailing list, please send a note to Darcy Sucevich (darcy.sucevich@contr.netl.doe.gov). Thank you.
Paula Turner



Boston Scientific prototype of a coronary stent.

ASM International Honors NETL Work on Platinum-Chromium Alloy for Coronary Stents

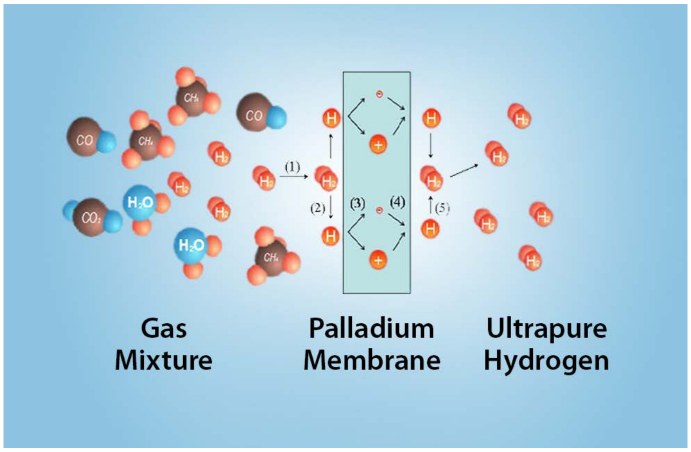
—The international materials science and engineering society ASM International will present a 2015 ASM Engineering Materials Achievement Award to NETL and its partner Boston Scientific along with the other organizations that worked on the development, transfer, and successful commercialization of a novel platinum-chromium alloy used in the manufacture of the next generation of coronary stents.

NETL scientists Paul Jablonski, Paul Turner, Edward Argetsinger (URS contractor), and Jeffrey Hansen (retired), as well as their collaborators from Boston Scientific Corporation, Carpenter Specialty Alloys, Minitubes, and Accellent, developed the alloy as the first stainless steel formulation for stents with a significant concentration of an element that is highly visible on X-ray: platinum. The platinum makes it easier for coronary specialists to see the stent during placement and expansion. The alloy also increases the stents' corrosive resistance, strength, and flexibility. The series benefits patients by shortening recovery time and avoiding follow-on procedures and more invasive surgery, which reduces healthcare costs. Since its introduction in 2010, the platinum-chromium stent series has generated more than $6 billion in sales and has captured a 25% U.S. share and a significant global share of the coronary stent market. Engineered and manufactured in the United States, it has created 450 sustainable, domestic jobs.

The ASM Engineering Materials Achievement Award has recognized outstanding materials science advancements since its inception in 1969. NETL will receive the award—our first time accepting this honor—at the ASM Awards dinner at the 2015 Materials Science and Technology meeting in Columbus, OH.

In winning the award, NETL joins the ranks of Lockheed Aircraft Corporation, Ford Motor Company, General Electric, Texas Instruments, Inc., and other innovation giants.

Contact: Paul C. Turner, 541-990-0204



Simple schematic of a hydrogen separation palladium (Pd) membrane.

Metallic Membranes Could be Key to Transforming Coal Syngas into Clean Hydrogen—Scientists at the National Energy Technology Laboratory (NETL) are leading an effort to find metallic membranes that can help create clean hydrogen from coal-derived syngas by filtering out undesirable gases like carbon dioxide (CO_2).

Hydrogen is used to hydrogenate oils, crack heavy hydrocarbons into lighter ones for fuels or chemical precursors, and, when very pure, generate power in fuel cells. It is an element rarely found on its own in nature—it must be manufactured by separating it out of compounds. Hydrogen can be produced when coal is gasified to generate hot syngas. But syngas also contains methane, carbon monoxide, CO_2, and smaller amounts of components like sulfur, arsenic, and selenium compounds. To use syngas as a source of hydrogen, separation membranes are needed that allow the hydrogen to pass through while other gases are kept out.

Dirk Link, technical coordinator for the NETL Fuels team, explained that metallic membranes are a promising approach to hydrogen separation at high temperatures. He said a research goal is to identify specific metals that help hydrogen gas dissociate into hydrogen atoms and then travel through the membrane's crystal structure before recombining on the other side as a pure hydrogen gas stream.

He said that unfortunately, minor syngas components such as hydrogen sulfide, arsine, and hydrogen selenide corrode most metallic membranes and hamper both dissociation of hydrogen gas and transport of hydrogen atoms through the membranes, often causing the whole system to fail.

To tackle the corrosion problem, the team is studying membranes made of various combinations of metals, as well as minor additions of other elements to improve performance—how well hydrogen is transported through the metal membrane—while increasing corrosion resistance and reducing overall cost. Link reports that the results are promising, but plenty of work is still to be done.

According to researcher Bret Howard, NETL is well-equipped to lead the search for the most effective metallic membranes. More than a decade ago, its researchers developed the capability to handle hydrogen gas at temperatures and pressures found in syngas cleanup systems. When interest in coal gasification led to a need for separation membrane development, the laboratory's capabilities were adapted to test membrane materials. Eventually, outside research labs began sending membrane materials to NETL for performance evaluation and assistance.

NETL expertise in alloy development, engineering, materials testing, and corrosion was eventually combined to form the NETL Fuels research team, which also includes URS Corporation researchers at NETL, industry partner Gasification Technologies, Inc. (GTI), the National Carbon Capture Center, and researchers from Carnegie Mellon University.

NETL's history of membrane testing, and the partnerships incorporated into the research team, will help move membrane technology further toward the goal of clean hydrogen fuel from syngas

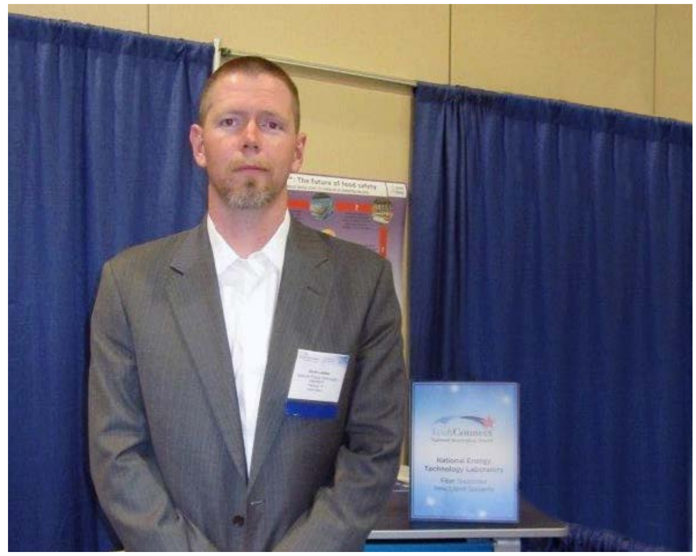
Contact: Dirk Link, 412-386-5765

Photo of the High Pressure Combustion laboratory.

Pressure Gain Combustor Completed and Ready for Testing

—NETL researchers have completed the design, fabrication, and installation of a rotating detonation-wave combustor (RDC) to be tested at elevated pressure in the NETL high-pressure combustion facility in Morgantown, WV. The RDC concept is being explored since it has the potential to improve gas turbine cycle efficiency by producing a significant pressure gain across the combustion section of a gas turbine – instead of the pressure loss typical of current state-of-the-art combustion systems. This efficiency improvement has the potential to reduce fuel consumption and subsequently carbon dioxide emissions. Researchers from NETL worked with colleagues at the Air Force Research Laboratory (AFRL) to modify their existing RDC design for high-pressure testing at the NETL facility. This collaboration with AFRL, the Naval Post-graduate School (NPS), and private companies to explore this potentially transformative concept is leveraging the research experience of these entities with NETL's unique combustion and diagnostic capabilities. Integration of the RDC into the NETL facility is continuing with instrumentation, control and safety system modifications; initial testing is planned for latter part of fiscal year 2014.

Contacts: Don Ferguson, 304-285-4192, and Todd Sidwell, 304-285-5452



David Luebke at the 2014 TechConnect National Innovation Showcase event

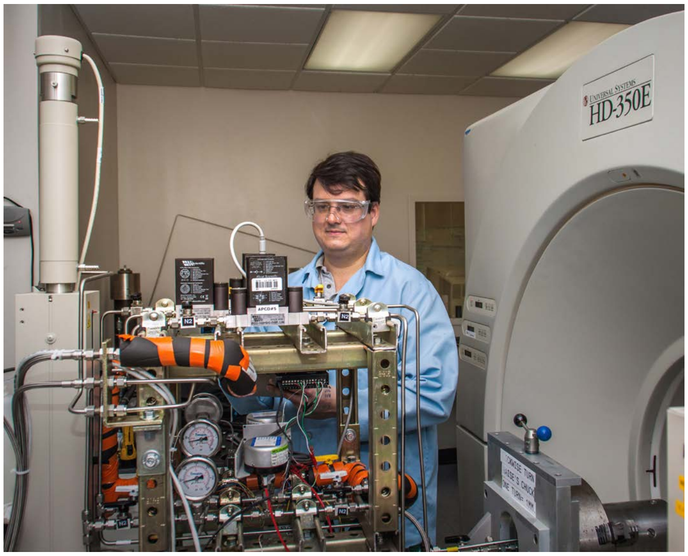
NETL Researchers Recognized for Innovative Technology Development

—In recent years, scientists and engineers including those at NETL have created a wide variety of new liquid materials which selectively absorb certain gases. The selective absorption of carbon dioxide is of particular importance to mitigate global climate change. A major problem with many of these liquids is their high viscosity. NETL researchers have developed a method for supporting these viscous liquids in polymer fibers, which avoids this problem by fixing the liquids in a permanent structured bed.

Conventional gas-liquid contactors cannot be used, which increases the expense of employing the liquids for gas separations. Ionic liquids—liquid organic salts at room temperature—are transformed into high surface area fiber material that can filter out impurities like CO_2, sulfur, and water from gas mixtures, paving the way for cheaper and more efficient gas separation in areas like natural gas reforming, carbon capture, and chemical manufacturing.

A patent has been granted for this technology, along with two additional patents pending, and industrial partners are being sought for its commercialization. This important work was presented at the TechConnect National Innovation Showcase in Washington, D.C., in June, where Dave Luebke's team was recognized with a National Innovation Award for "Fiber Supported Ionic Liquid Sorbents."

Contact: Dave Luebke, 412-386-4118



Dustin McIntyre works with the medical CT scanner at the CT Imaging Facility at the National Energy Technology Laboratory in Morgantown, WV.

Laser-Induced Breakdown Spectroscopy for Carbon Dioxide Leak Detection

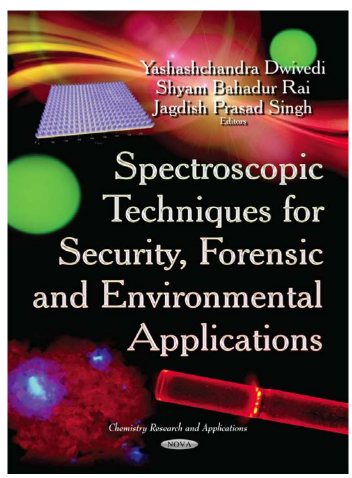
—A new laser-induced breakdown spectroscopy (LIBS) system, developed by NETL researcher Dustin McIntyre, will enable monitoring of downhole fluids to detect chemistry changes indicative of CO_2 migration. The system will play a key role in investigating storage permanence related to carbon capture, utilization, and storage (CCUS), and will help to ensure that injected CO_2 remains in its intended underground repository.

The system uses a remotely positioned laser diode coupled to an optical fiber. The light from the diode travels through the optical fiber where it is then focused into a monolithic laser gain medium to form an end-pumped laser system, which is similar to a high-powered green laser pointer. The light delivered by the fiber excites a passively Q-switched laser, which produces a high-peak power pulse that is directed at a location of interest. The light from the spark is then collected for spectral analysis.

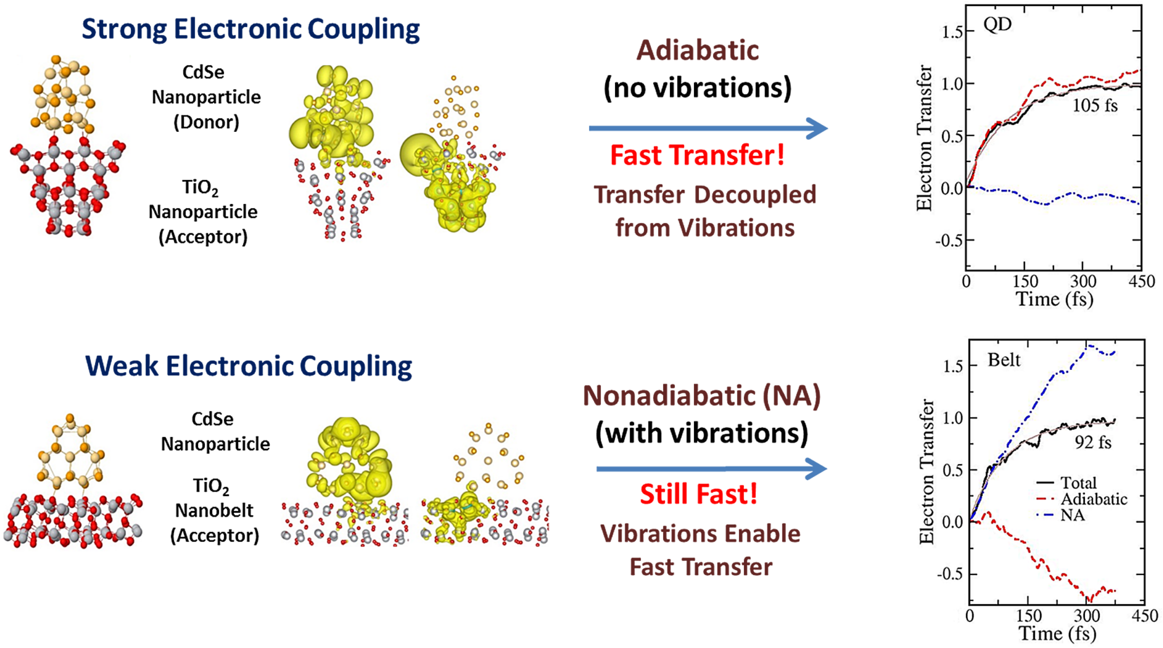
What makes McIntyre's system unique is the remotely positioned laser diode pump, compared to other technologies that require complete laser systems to deliver high-peak energy. The separation of the pump source allows the low-peak power pumping pulse to be delivered to a remotely located solid-state laser where the high-peak pulse is produced. If the high-peak power pulse required to produce the laser spark was coupled to an optical fiber, the optical breakdown threshold of the fiber would be exceeded and the fiber would be seriously damaged. When using Raman excitation to evaluate molecular species, a split laser system can be advantageous. By producing the Raman probe signal at a remote location, the system avoids the Raman emission signal that would be produced by the optical fiber delivery system. Monitoring devices, such as McIntyre's LIBS system, placed around an injection site would enable researchers to detect the presence of leachates from the original formation.

With this information, researchers would be able to determine if the injected CO_2 is migrating into other formations where it could potentially impact ground water. Currently, McIntyre's research team is fabricating a prototype sensor for demonstration. They're also designing an LIBS system that comprises multiple lasers, which would be distributed over a wide area to enable multiple monitoring locations over a CO_2 storage site. Moving forward, the team's primary challenges will be keeping up with the cost of the technology, which is rapidly decreasing, as well as the adoption of new components, which are becoming more and more accessible.

Dr. McIntyre's work was featured in an interview appearing in the March 14, 2014 edition of Spectroscopy magazine (available online). His team also recently contributed a book chapter on LIBS, with topics ranging from CO_2 sensing in air to total carbon measurement in soil and measurements on calcium and potassium in a sodium-rich solution. (Citation: McIntyre, D.L., Jain, J.C., Goueguel, C.L., Singh, J.P., "Application of Laser Induced Breakdown Spectroscopy (LIBS) to Carbon Sequestration Research and Development," Spectroscopic Techniques for Security, Forensic, and Environmental Applications, pp. 25-51, Nova Science Publishers, 2014, ISBN: 978-1-63117-4)



Contact: Dustin McIntyre, 304-285-1374



Mechanism of photoinduced electron injection from a CdSe nanoparticle to TiO_2 nanoparticle and TiO_2 nanobelt.

How Do the Size, Shape, and Atomic Vibrations of Catalysts Influence CO_2 Conversion?

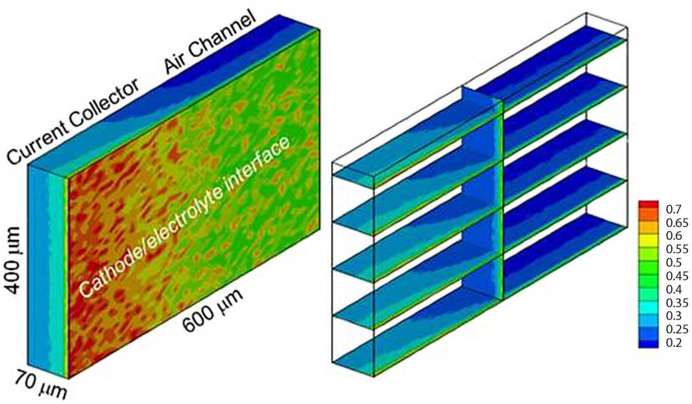
—A research team has taken a deep dive into the mysteries of how the atomic vibrations present in different sizes and shapes of catalytic elements can vary the chemical reactions in a process that converts carbon dioxide (CO_2) into usable gases and fuels. The theoretical work of researchers at NETL, the University of Rochester, and the University College Dublin is determining how electrons are passed between cadmium selenide (CdSe) quantum dots and nanocrystalline titanium dioxide (TiO_2), and then used to reduce CO_2 to methane and methanol. These materials were previously demonstrated at NETL as the first-ever, visible-light active CO_2-utilization photocatalysts, but they are also widely used in photovoltaic and electronic applications. A photocatalyst is a light-absorbing substance, which, when added to a reaction, accelerates the reaction while remaining unchanged at the end of the reaction.

The relationship between lattice vibrations and the size and shape of catalysts has been so complex that scientists have simply ignored it, even in computational simulations. In fact, one of the most fundamental approximations in the chemical sciences, the Born-Oppenheimer approximation, which allows the wave function of a molecule to be broken into its electronic and nuclear components, addresses this technical challenge by completely neglecting the influence of vibrations on electron behavior. Only recently have researchers at the University of Rochester developed methods to move beyond the Born-Oppenheimer approximation and, through collaboration with NETL researchers, applied them to CO_2 utilization.

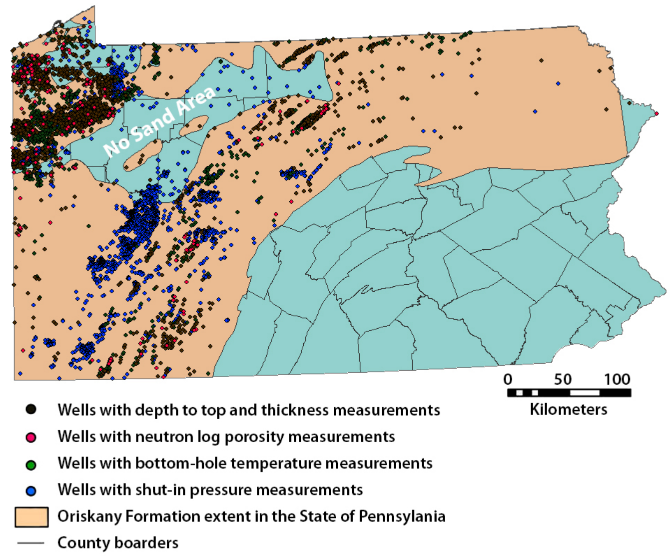
A strong electronic coupling between CdSe and spherical TiO_2 nanoparticles leads to facile, excited-state electron transfer without the need to dissipate excess energy through lattice vibrations. In comparison, electronic coupling between CdSe and TiO_2 nanobelts (belt-like shape nanocrystals) is weak, which would normally lead to slow electron transfer. However, symmetry breaking due to the size and shape of this system creates new relaxation pathways and allows for facile electron transfer by dissipating energy to lattice vibrations (phonons).

This research will shed light on the role electron transfer plays in the speed and efficiency of reducing CO_2 to usable gases and fuels. It also provides radical new insight into materials design for photocatalysis, photovoltaics and other applications where electron transfer is a critical rate-determining step toward performance. Read more about this research in Nano Letters.

Contact: Denyago Tafen, 541-918-4462



Fundamental computations (3D multi-physics model) inform modeling of advanced degradation, performance, and microstructural evolution at the cell and stack level.



NETL Project Receives Maximum Score in Solid Oxide Fuel Cell Program Peer Review—NETL's Fuel Cell project received the maximum score of 10 from peer reviewers evaluating DOE's Solid State Energy Conversion Alliance (SECA) Program. In generating the evaluation, the peer review team considered the project's technical scope, technical accomplishments/productivity, program relevance, project benefits and potential for commercial impact, and resource management. Reviewers identified nine major strengths and two minor strengths, and commended the team for its technical quality, efforts to engage industrial partners, integration of the management plan and approach, and effectiveness in coordinating team members' skills among various research priorities. SECA is DOE's principal solid oxide fuel research program, and coordinates development activities among national laboratories, industrial developers, and universities. The peer review was conducted April 16 and 17, 2014 and reviewer scores were provided to projects on May 15.

Future work will focus on localized degradation and a more complete failure analysis along with an economic study.

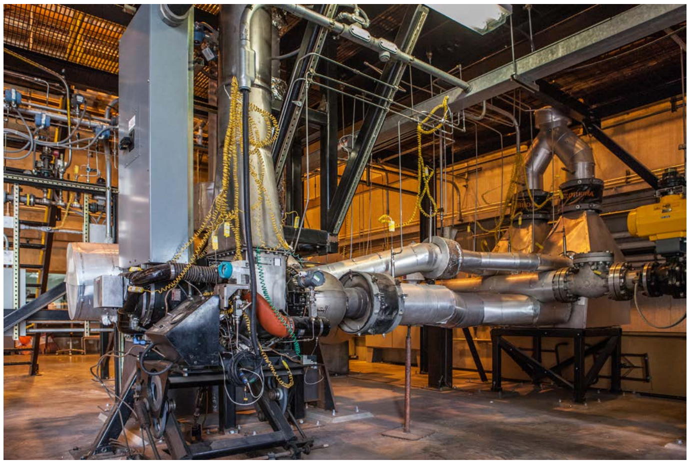
Contact: Kirk Gerdes, 304-285-4342

NETL Develops Geospatial Stochastic Model to Assess CO_2 Storage—In collaboration with partners from Carnegie Mellon University and the University of Pittsburgh, this work introduces a geostatistical model developed to estimate the CO_2 storage resource in sedimentary formations. The Oriskany Formation of the Appalachian sedimentary basin in Pennsylvania is used as a case study for model implementation. This model is constructed using four separate datasets provided by the Pennsylvania Bureau of Topographic & Geologic Survey (BTGS). These datasets contain records on wells installed in Pennsylvania by different industry operators.

The proposed stochastic model is based on Sequential Gaussian Simulation and accounts for the spatial distribution of reservoir properties such as thickness, porosity, and CO_2 density. Results indicate that the CO_2 storage resource for the Pennsylvania portion of the Oriskany Formation has substantial spatial variation due to heterogeneity of formation properties and basin geology leading to uncertainty in the storage assessment.

The methodology can be applied to other sedimentary formations to forecast geospatial trends and estimate CO_2 sequestration storage and uncertainty. More precise CO_2 storage resource estimates will provide better recommendations for government and industry leaders and inform their decisions on which greenhouse gas mitigation measures are best fit for their regions.

Contact: Angela Goodman, 412-386-4962



NETL's Hybrid Performance, or Hyper, facility is a one-of-a-kind laboratory.

Hybrid Gas Turbine System Control Strategy Greatly Extends Fuel Cell Life

—Using an appropriate control strategy, the life expectancy of a solid oxide fuel cell (SOFC) was found to be extended by ten times when coupled with a gas turbine in a hybrid configuration, compared to a standalone configuration. This extended lifetime could position fuel cell-based systems to compete economically with other power generation technology.

Fuel cells' power output degrades gradually over time due to cell losses. A recently completed Lifetime Assessment concluded that the performance of a standalone fuel cell system degraded nearly 35 times faster than a fuel cell in a hybrid gas turbine system using appropriate controls system when both were operated at constant power output.

Accelerated aging tests conducted in the HyPer test facility at NETL confirmed this dramatic result. The HyPer facility dynamically couples what we know about fuel cell degradation and performance with turbine hardware by coupling the fuel cell responses such as pressure fluctuations, heat, and mass flows from a real-time model to the input of a real, high-temperature gas turbine. The result is a real-time fuel cell model imbedded in the hardware of a hybrid power system loop.

In order to assess the long-term stability of the SOFC part of the system, electrochemical degradation due to operating conditions such as current density and fuel utilization were incorporated into the HyPer facility's SOFC model and successfully recreated in real time for standalone and hybrid operation.

Researchers customized the HyPer facility to simulate degradation in real time using novel advanced control systems. Upon initiation of degradation, researchers used a proportional integral derivative (PID) controller to maintain constant fuel cell power by increasing total fuel cell current as the voltage dropped off. The PID controller added fuel to the fuel cell to maintain constant fuel utilization as the fuel cell voltage and corresponding power decreased. The PID controller continued to increase current to maintain a constant power.

As degradation occurred in the hybrid configuration, the additional heat from the fuel cell was partially recovered in the turbine, offsetting the losses in output. Fuel utilization decreased in the SOFC over the period of degradation as additional fuel was added to increase turbine load. The lower fuel utilization resulted in a lower degradation rate over time, and a higher Nernst potential, counteracting the voltage drop from degradation.

While SOFC turbine hybrid power systems are one of the most efficient power generation technologies available, high SOFC replacement costs have stifled development. However, reducing SOFC replacement by an order of magnitude enables the fuel cell-based system to compete with any other power generation technology, but with higher efficiency and less emissions.

This experimental work has been accepted for publication in the *Journal of Fuel Cell Science and Technology*. The Lifetime Assessment will be presented at the 2014 ASME 8th International Conference on Energy Sustainability and 12th Fuel Cell Science, Engineering and Technology Conference in Boston this summer, and the manuscripts will be published in the conference proceedings.

Contact: David Tucker, 304-285-4182

Recent NETL Publications

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Patents Issued This Quarter

1.	Basic Refractory and Slag Management for Petcoke Carbon Feedstock in Gasifiers, Kyei-Sing Kwong; James P. Bennett (DOE/NETL); Jinichiro Nakano (URS); **8703021**, issued April 22, 2014.
2.	Nanocomposite Thin Films for Optical Gas Sensing, Thomas Brown (DOE/NETL); Paul Ohodnicki, Jr. (DOE/NETL), **8741657**, issued June 3, 2014.

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